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memorandum

TO: J. R. Streetman, N–12, MS K551

FROM: R. E. Seamon, X–6

DATE: 15–May–1992

MAIL STOP/TELEPHONE: B226 / 7–4809

SYMBOL: X–6:RES–92–324

SUBJECT: Revised ENDF/B–V Zirconium Cross Sections

Last Friday – literally one week ago – you called me about an error encountered with the Monte Carlo code MCNP (Ref. 1) when you used the ENDF/B–V zirconium cross sections under ZAID=40000.50C. A fatal error was encountered with MT=91, Law 9.

This problem had been encountered at least twice before, as documented in Ref. 2. There is an error in the value of U used in the Law 9 evaporation spectrum in terms of which the secondary neutrons for the (n,n′)C (MT=91) reaction is described; the value of U in ENDF/B–V MAT=1340 for MT=91 is 2.871 MeV and should be 2.821 MeV. This accounts for the problem in the incident neutron energy range 2.852MeV $\leq E_n \leq$ 2.871 MeV.

Five new cross–section sets for ZA=40000 have been prepared with the U value changed from 2.871 MeV to 2.821 MeV. The correlation between current and revised ZAIDs is as follows:

Current ZAID	Revised ZAID	Temperature (°K)
40000.51C	40000.57C	300.0
40000.51D	40000.57D	300.0
40000.50C	40000.56C	300.0
40000.50D	40000.56D	300.0
40000.53C	40000.58C	600.0

In answer to your call for help last Friday, a Type 1 BCD cross–section set was prepared for ZAID=40000.56C and a one–line directory was also provided. You have transferred that BCD file to your Sun workstation environment. That, it turns out, is the final solution to the problem. We do not intend to change U on the plethora of cross–section libraries that exist.

You asked me whether this change would invalidate results previously obtained using ZAID = 40000.50C. My answer then and now is NO, but it is understood that problems using ZAID=40000.50C and ZAID=40000.56C cannot be expected to track because U plays a role in the Law 9 expression; *viz.*,

$$f(E \rightarrow E') = \frac{E'}{I} e^{-\frac{E'}{T(E)}}$$

with restriction $0 \leq E' \leq E - U$ and

$$I = T^2(E)\left[1 - e^{-\frac{E-U}{T(E)}}\left(1 + \frac{E-U}{T(E)}\right)\right].$$

However, the (n,n′)C reaction is at most about a third of the total cross section in the energy range 1.0 to 20.0 MeV as shown in Figs. 1 and 2 and in Table I. I am not worried about the validity of the MCNP runs you have made with ZAID=40000.50C, but urge you to use ZAID=40000.56C henceforth.

REFERENCES

1. J. F. Briesmeister, Ed., "MCNP – A General Monte Carlo Code for Neutron and Photon Transport, Version 3A," Los Alamos National Laboratory manual LA–7396–M, Rev. 2 (September 1986).
2. R. E. Seamon, "Repairing ENDF/B–V Zirconium Cross Sections," Los Alamos National Laboratory internal memorandum X–6:RES–91–358 to R. C. Little (June 20, 1991).

DISTRIBUTION

R. C. Little, X–6, MS B226
R. E. H. Clark, X–6, MS B226
X–6 Files, MS B226 (2)

RES:res

Table I

Multigroup Comparison of (n,n′)C Cross Section to Total Cross Section for ENDF/B–V Zirconium Evaluation

g	Energy Boundaries (MeV)	$< \sigma_{MT=91} >_g / < \sigma_{MT=1} >_g$
9	2.232–2.865	1.7×10^{-6}
8	2.865–3.680	0.034
7	3.680–6.070	0.203
6	6.070–7.790	0.328
5	7.790–10.0	0.321
4	10.0–12.0	0.252
3	12.0–13.5	0.197
2	13.5–15.0	0.140
1	15.0–17.0	0.081

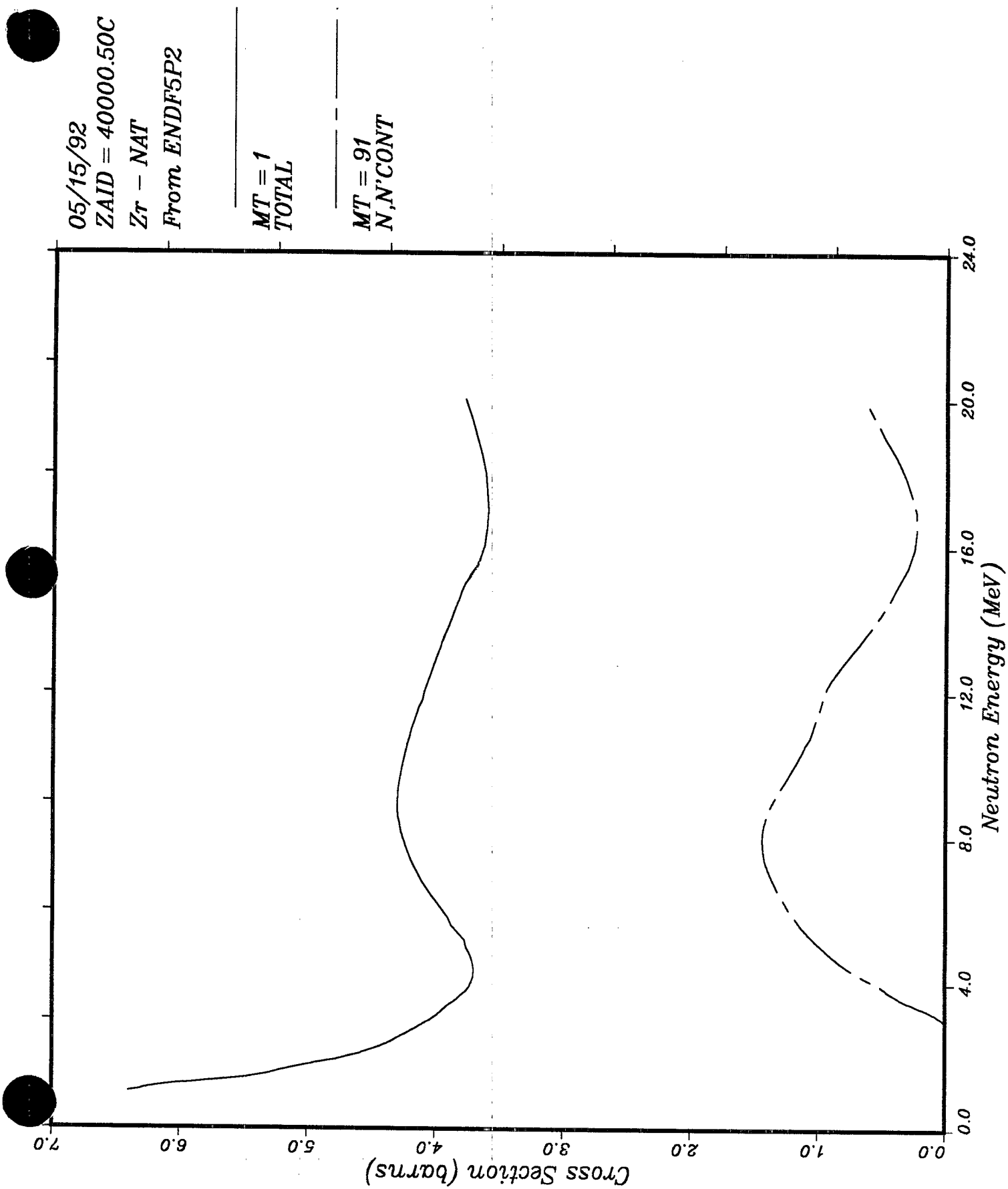
05/15/92
ZAID = 40000.50C
Zr – NAT
From ENDF5P2
MT = 1
TOTAL
MT = 91
N,N'CONT
Cross Section (barns)
Neutron Energy (MeV)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
0.0
4.0
8.0
12.0
16.0
20.0
24.0

Figure 1

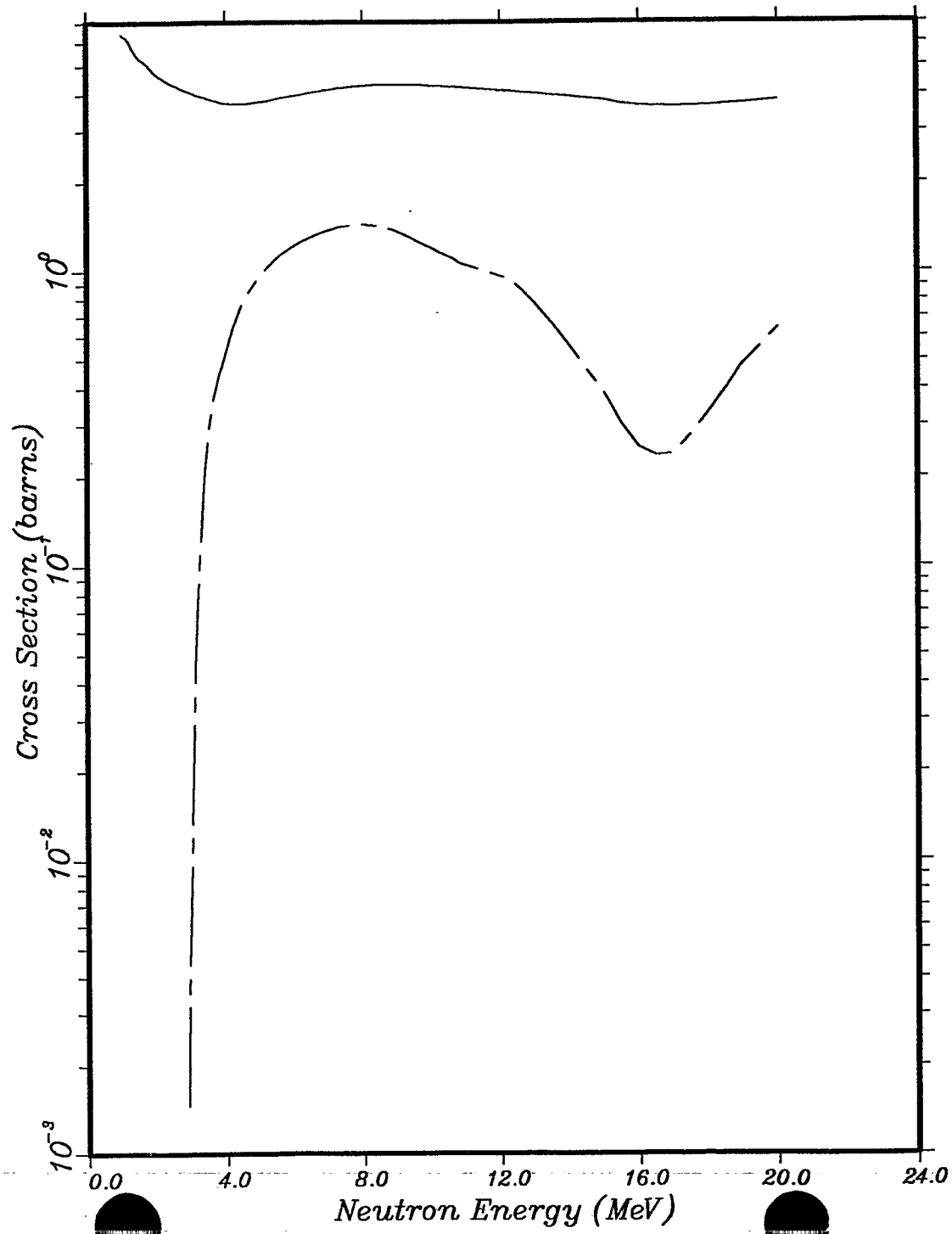
05/15/92
ZAID = 40000.50C
Zr – NAT
From ENDF5P2
MT = 1
TOTAL
MT = 91
N,N'CONT
Cross Section (barns)
10^{0}
10^{-1}
10^{-2}
10^{-3}
0.0
4.0
8.0
12.0
16.0
20.0
24.0
Neutron Energy (MeV)

Figure 4